

## Author Index of Volume 74

- |                      |                    |                     |                      |
|----------------------|--------------------|---------------------|----------------------|
| Abu Al-Rub, F.A. 205 | Dai, G.Q. 211, 217 | Kärger, J. 15       | Pal, S. 77           |
| Alexander, P. 57     | Do, D.D. 155       | Kakaç, S. 147       | Pimentel, L.C.G. 147 |
| Auerbach, S.M. 43    |                    | Keffer, D. 33       |                      |
|                      | Fichthorn, K.A. 77 | Kioupis, L.I. 129   | Rao, K.K. 161        |
| Balasundaram, R. 117 | Flamant, G. 181    |                     | Roberts, B.W. 67     |
| Banat, F.A. 205      |                    | Li, J.M. 211, 217   | Rutherford, S.W. 155 |
| Belak, J. 117        | Gauthier, D. 181   | Lin, J. 99          |                      |
| Ben-Shebil, S.M. 197 | Gladden, L.F. 57   | Luo, W. 67          | Šolcová, O. 171      |
| Boyle, M.J. 85       |                    |                     | Sastri, S.R.S. 161   |
|                      | Haberlandt, R. 15  | MacElroy, J.M.D. 85 | Schneider, P. 171    |
| Čapek, P. 171        | Hargreaves, M. 57  | Maginn, E.J. 129    | Sholl, D.S. 25       |
| Chen, W.M. 211, 217  | Hejtmánek, V. 171  | McCormick, A.V. 1   | Simandl, J. 205      |
| Chu, L.Y. 211        |                    | Mohanty, S. 1       |                      |
| Clancy, P. 67        | Jiang, S. 117      | Murad, S. 99        | Yethiraj, A. 109     |
| Cotta, R.M. 147      | Johnson, K.A. 67   | Nelson, P.H. 43     | Zerguerras, S. 181   |



## Subject Index of Volume 74

- Adsorbate passage  
Characterizing adsorbate passage in molecular sieve pores, 25
- Adsorbate  
Molecular dynamics under the confinement by the host lattice in zeolitic adsorbate–adsorbent systems, 15
- Adsorbent  
Molecular dynamics under the confinement by the host lattice in zeolitic adsorbate–adsorbent systems, 15
- Adsorption  
Effect of heat of adsorption on the adsorptive drying of solvents at equilibrium in a packed bed of zeolite, 197
- Alkanes  
Rheology, dynamics, and structure of hydrocarbon blends: a molecular dynamics study of *n*-hexane/*n*-hexadecane mixtures, 129
- Anisotropic zeolite membranes  
Modeling tracer counter-permeation through anisotropic zeolite membranes: from mean field theory to single-file diffusion, 43
- Asymmetric  
Fully developed turbulent flow in ducts with symmetric and asymmetric rough walls, 147
- Carbon membranes  
Nonequilibrium molecular dynamics simulation of a model carbon membrane separation of CH<sub>4</sub>/H<sub>2</sub> mixtures, 85
- Complete fluidization velocity  
Influence of the particle size distribution of powders on the velocities of minimum and complete fluidization, 181
- Computer simulation  
Molecular modeling of polymers at surfaces, 109
- Concentration  
Experimental study of solid–liquid two-phase flow in a hydrocyclone, 211
- Confined fluid  
Structural and rheological properties of *n*-decane confined between graphite surfaces, 117
- Counter-permeation  
Modeling tracer counter-permeation through anisotropic zeolite membranes: from mean field theory to single-file diffusion, 43
- Critical temperature  
A new temperature–thermal conductivity relationship for predicting saturated liquid thermal conductivity, 161
- Density functional theory  
Molecular modeling of polymers at surfaces, 109
- Drying  
Effect of heat of adsorption on the adsorptive drying of solvents at equilibrium in a packed bed of zeolite, 197
- Dusty-gas model  
Dynamics of pressure build-up accompanying multicomponent gas transport in porous solids: adsorbable gases, 171
- Dynamic transport  
Dynamics of pressure build-up accompanying multicomponent gas transport in porous solids: adsorbable gases, 171
- Flow field  
Numerical prediction of the liquid flow within a hydrocyclone, 217
- Further equation  
Isothermal vapour–liquid equilibria of 1-propanol–water–salt mixtures, 205
- Gas-solid fluidization  
Influence of the particle size distribution of powders on the velocities of minimum and complete fluidization, 181
- Grand canonical Monte Carlo  
Monte Carlo lattice dynamics studies of binary adsorption in silicalite, 57
- Heat effects  
Effect of heat of adsorption on the adsorptive drying of solvents at equilibrium in a packed bed of zeolite, 197
- Hydrocyclone  
Experimental study of solid–liquid two-phase flow in a hydrocyclone, 211  
Numerical prediction of the liquid flow within a hydrocyclone, 217
- Integral equation theory  
Molecular modeling of polymers at surfaces, 109
- Intrinsic defect diffusion  
An order(*N*) tight-binding molecular dynamics study of intrinsic defect diffusion in silicon, 67
- Kinetic Monte-Carlo  
Modeling tracer counter-permeation through anisotropic zeolite membranes: from mean field theory to single-file diffusion, 43
- Liquid phase  
Effect of heat of adsorption on the adsorptive drying of solvents at equilibrium in a packed bed of zeolite, 197
- Lubricants  
Rheology, dynamics, and structure of hydrocarbon blends: a molecular dynamics study of *n*-hexane/*n*-hexadecane mixtures, 129
- Mass transfer rates  
Molecular modeling of fluid separations using membranes: effect of molecular forces on mass transfer rates, 99
- Mean field theory  
Modeling tracer counter-permeation through anisotropic zeolite membranes: from mean field theory to single-file diffusion, 43
- Mean transport pore model  
Dynamics of pressure build-up accompanying multicomponent gas transport in porous solids: adsorbable gases, 171
- Method of calculation  
A new temperature–thermal conductivity relationship for predicting saturated liquid thermal conductivity, 161
- Minimum fluidization velocity  
Influence of the particle size distribution of powders on the velocities of minimum and complete fluidization, 181

## Mixture

Rheology, dynamics, and structure of hydrocarbon blends: a molecular dynamics study of *n*-hexane/*n*-hexadecane mixtures, 129

## Molecular dynamics

Molecular dynamics under the confinement by the host lattice in zeolitic adsorbate-adsorbent systems, 15

Molecular modeling of fluid separations using membranes: effect of molecular forces on mass transfer rates, 99

Monte Carlo lattice dynamics studies of binary adsorption in silicalite, 57

Rheology, dynamics, and structure of hydrocarbon blends: a molecular dynamics study of *n*-hexane/*n*-hexadecane mixtures, 129

Structural and rheological properties of *n*-decane confined between graphite surfaces, 117

## Molecular sieve pores

Characterizing adsorbate passage in molecular sieve pores, 25

## Molecular-dynamic (MD) simulation

Accelerated molecular dynamics of infrequent events, 77

## Monte Carlo (MC) simulation

Accelerated molecular dynamics of infrequent events, 77

## Monte Carlo lattice dynamics

Monte Carlo lattice dynamics studies of binary adsorption in silicalite, 57

## Multicomponent

Dynamics of pressure build-up accompanying multicomponent gas transport in porous solids: adsorbable gases, 171

## Nanopores

The temperature dependence of single-file separation mechanisms in one-dimensional nanoporous materials, 33

## Nonequilibrium molecular dynamics

Nonequilibrium molecular dynamics simulation of a model carbon membrane separation of  $\text{CH}_4/\text{H}_2$  mixtures, 85

## Normal boiling point

A new temperature-thermal conductivity relationship for predicting saturated liquid thermal conductivity, 161

## Numerical simulation

Numerical prediction of the liquid flow within a hydrocyclone, 217

## One-dimensional

The temperature dependence of single-file separation mechanisms in one-dimensional nanoporous materials, 33

## Organic liquids

A new temperature-thermal conductivity relationship for predicting saturated liquid thermal conductivity, 161

## Particle size distribution

Influence of the particle size distribution of powders on the velocities of minimum and complete fluidization, 181

## Particle size

Experimental study of solid-liquid two-phase flow in a hydrocyclone, 211

## Particle-particle interaction

Influence of the particle size distribution of powders on the velocities of minimum and complete fluidization, 181

## Permeation

Nonequilibrium molecular dynamics simulation of a model carbon membrane separation of  $\text{CH}_4/\text{H}_2$  mixtures, 85

## Potential-energy surface

Accelerated molecular dynamics of infrequent events, 77

## Rheology

Rheology, dynamics, and structure of hydrocarbon blends: a molecular dynamics study of *n*-hexane/*n*-hexadecane mixtures, 129

Structural and rheological properties of *n*-decane confined between graphite surfaces, 117

## Rough walls

Fully developed turbulent flow in ducts with symmetric and asymmetric rough walls, 147

## Semi-permeable membranes

Molecular modeling of fluid separations using membranes: effect of molecular forces on mass transfer rates, 99

## Silicon

An order(*N*) tight-binding molecular dynamics study of intrinsic defect diffusion in silicon, 67

## Simulation

Prospects for principles of size and shape selective separations using zeolites, 1

## Single-file diffusion

Modeling tracer counter-permeation through anisotropic zeolite membranes: from mean field theory to single-file diffusion, 43

## Size and shape selective separations

Prospects for principles of size and shape selective separations using zeolites, 1

## Solvents

Effect of heat of adsorption on the adsorptive drying of solvents at equilibrium in a packed bed of zeolite, 197

## Symmetric

Fully developed turbulent flow in ducts with symmetric and asymmetric rough walls, 147

## Temperature dependence

The temperature dependence of single-file separation mechanisms in one-dimensional nanoporous materials, 33

## Thermal conductivity

A new temperature-thermal conductivity relationship for predicting saturated liquid thermal conductivity, 161

## Tight-binding molecular dynamics

An order(*N*) tight-binding molecular dynamics study of intrinsic defect diffusion in silicon, 67

## Tracer diffusion

Characterizing adsorbate passage in molecular sieve pores, 25

## Transition-state theory (TST)

Accelerated molecular dynamics of infrequent events, 77

## Transport parameters

Dynamics of pressure build-up accompanying multicomponent gas transport in porous solids: adsorbable gases, 171

## Turbulence

Numerical prediction of the liquid flow within a hydrocyclone, 217

## Turbulent flow

Fully developed turbulent flow in ducts with symmetric and asymmetric rough walls, 147

## Two-phase flow

Experimental study of solid-liquid two-phase flow in a hydrocyclone, 211

## Vapour-liquid equilibrium

Isothermal vapour-liquid equilibria of 1-propanol-water-salt mixtures, 205

## Velocity

Experimental study of solid-liquid two-phase flow in a hydrocyclone, 211

## Viscoelasticity

Rheology, dynamics, and structure of hydrocarbon blends: a molecular dynamics study of *n*-hexane/*n*-hexadecane mixtures, 129

## Zeolite

Effect of heat of adsorption on the adsorptive drying of solvents at equilibrium in a packed bed of zeolite, 197

## Zeolites

Prospects for principles of size and shape selective separations using zeolites, 1

